

ANSWERS: Reaction schemes

1) i) Reagent: NaBH_4 / LiAlH_4

Type of reaction – reduction / redox

ii) Reagent: conc H_2SO_4 / conc H_3PO_4 / Al_2O_3

Type of reaction – elimination / dehydration / condensation

iii) Explanation:

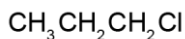
- An elimination reaction occurs because the molecule has changed from saturated to unsaturated / a ($\text{C}=\text{C}$) double bond forms.
- Because water is removed / H and OH have been removed (from adjacent C atoms).
- The but-2-ene is the major product / but-1-ene is the minor product.
- A mixture of products is formed, because the two carbons adjacent to the carbon-bearing OH have different numbers of H atoms attached / it is asymmetric.

(Zaitsev's rule – the major product has the more substituted double bond)

2) 1 SOCl_2

(Accept PCl_3 , PCl_5 or conc HCl / ZnCl_2)

B

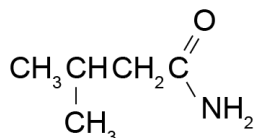


C



3) Name: 3 methyl butanoyl chloride.

Products:



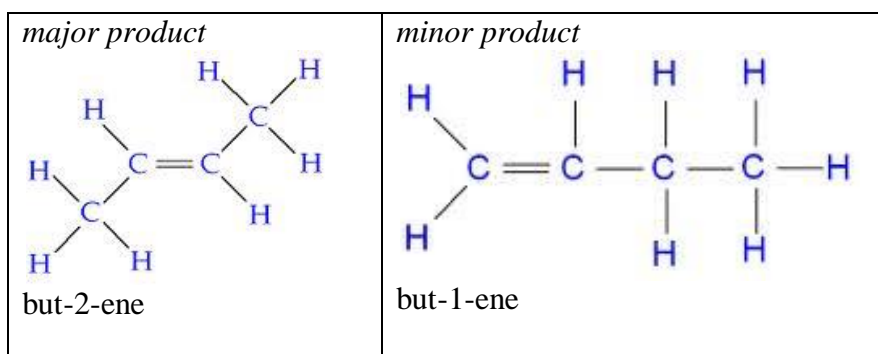
Hydrogen chloride / HCl / ammonium chloride / NH_4Cl

4) NaOH or KOH (alcoholic)

Elimination reaction

This is an elimination reaction as a hydrogen atom and a chlorine atom on adjacent carbon atoms are removed, forming a carbon-to-carbon double bond.

<p>5 a) Product A:</p> $\begin{array}{c} \text{H} & \text{H} & \text{H} & \text{O} \\ & & & // \\ \text{H}-\text{C} & -\text{C} & -\text{C} & -\text{C}-\text{O}-\text{H} \\ & & & \\ \text{H} & \text{H} & \text{H} & \end{array}$ <p style="text-align: center;">butanoic acid</p> <p>Product B:</p> $\begin{array}{c} \text{H} & \text{H} & \text{H} & \text{H} & \text{H} \\ & & & & \\ \text{H}-\text{C} & -\text{C} & -\text{C} & -\text{C} & -\text{O}-\text{H} \\ & & & & \\ \text{H} & \text{H} & \text{H} & \text{H} & \end{array}$ <p style="text-align: center;">butan-1-ol</p>	<p>Product C:</p> $\begin{array}{c} & \text{H} & \text{H} & \text{H} & \\ & & & & \\ \text{H} & & \text{C} = \text{C} & -\text{C} & -\text{C}-\text{H} \\ & & & & \\ & \text{H} & & \text{H} & \text{H} \end{array}$ <p style="text-align: center;">but-1-ene</p>
<p>b) Reactant 1 → no reaction</p> <p>Reactant 2 → butan-2-ol</p>	<p>Reactant 3 →</p> $\begin{array}{c} & & \text{H} & & \\ & & & & \\ & \text{H} & \text{H} & \text{O} & \text{H} \\ & & & & \\ \text{H}-\text{C} & -\text{C} & -\text{C} & -\text{C} & -\text{H} \\ & & & & \\ \text{H} & \text{H} & \text{H} & \text{H} & \end{array}$



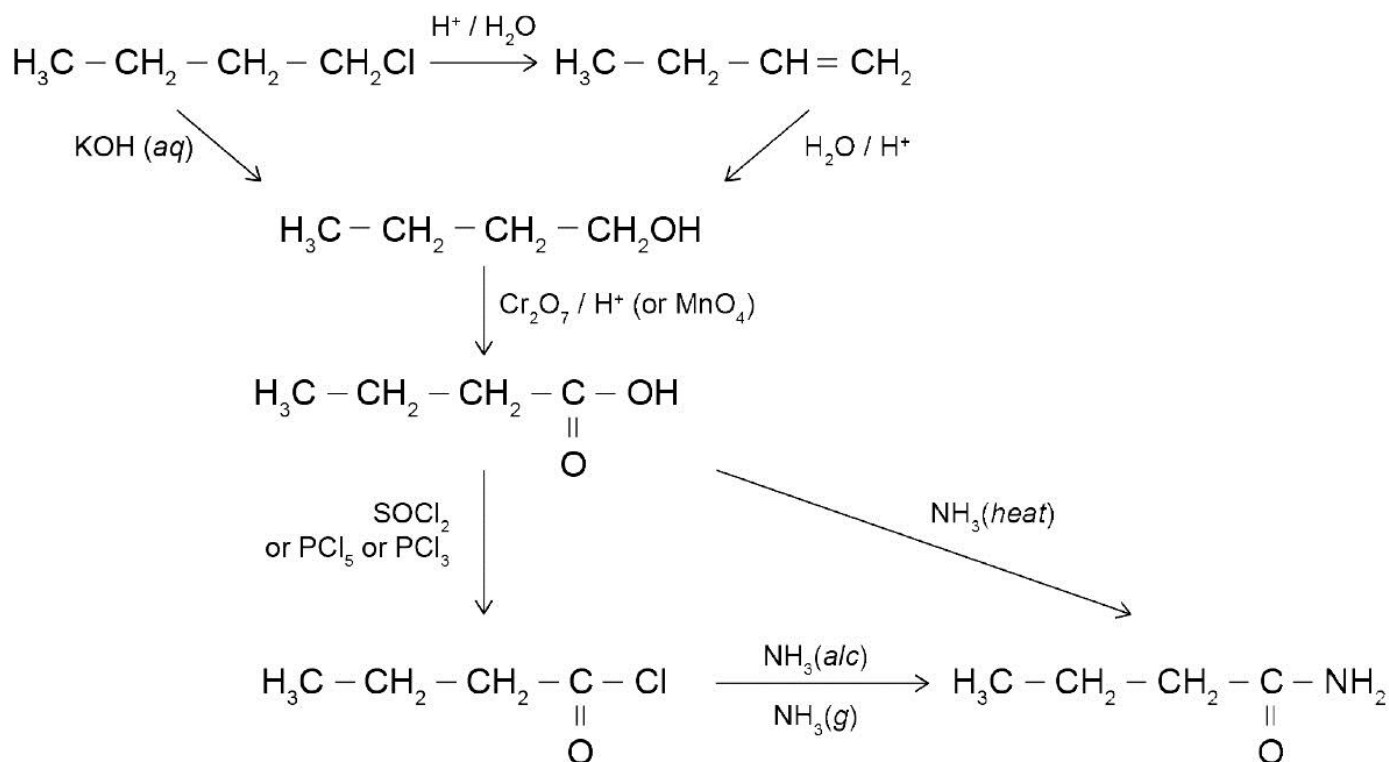
c) The two reaction schemes start with different compounds.

The first reaction starts with an aldehyde (butanal) which can be oxidised using $\text{Cr}_2\text{O}_7^{2-}$ (*reactant 1*) further to a carboxylic acid (butanoic acid). However, the ketone cannot be oxidised as the carbon atom with the double bond to the oxygen atom has no more hydrogen atoms bonded to it so will not be oxidised.

Both butanal/aldehydes and butanone/ketones can be reduced using NaBH_4 (Reactant 2) to form alcohols. In the second reaction both the schemes form an alcohol. But the first scheme produces a primary alcohol as that is what an aldehyde is derived from ie a primary alcohol is oxidised to form an aldehyde (butan-1-ol). While in the second scheme a secondary alcohol is produced as the ketone is derived from a secondary (butan-2-ol).

In the last reaction both the schemes form alkenes as conc H_2SO_4 reacts with alcohols to form alkenes. The first scheme forms 1 alkene as the last carbon loses the OH so the double bond can only form with the next carbon so but-1-ene is formed. While in the second scheme because the OH was on the second carbon there are two possible products the major product but-2-ene and the minor product but-1-ene. The major product will form.

6)

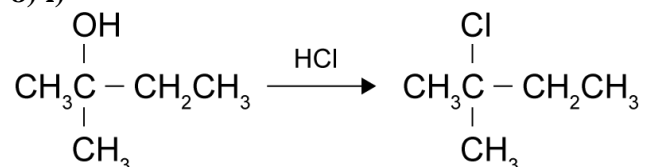


7)

A	Reagent 1 = NaOH(aq) Reagent 2 = NaOH(aq) ,
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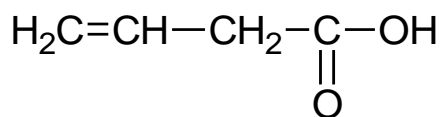
$\text{H}_3\text{C}-\text{CH}_2-\overset{\text{O}}{\underset{\text{O}-\text{CH}_2-\text{CH}_2-\text{CH}_3}{\text{C}}}=\text{O}$ <p>propyl propanoate B - sodium propanoate</p> <p>C</p> $\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{OH}$ <p>propan-1ol (1-propanol)</p> <p>D</p> $\text{H}_3\text{C}-\text{CH}_2-\overset{\text{O}}{\underset{\text{OH}}{\text{C}}}=\text{O} \quad \text{OR} \quad \text{H}_3\text{C}-\text{CH}_2-\overset{\text{O}}{\underset{\text{Cl}}{\text{C}}}=\text{O}$ <p>propanoic acid propanoyl chloride</p> <p>OR methylpropanoate</p> <p>E</p> $\text{H}_3\text{C}-\text{CH}_2-\overset{\text{O}}{\underset{\text{H}}{\text{C}}}=\text{O} \quad \text{OR} \quad \text{H}_3\text{C}-\text{CH}_2-\overset{\text{O}}{\underset{\text{OH}}{\text{C}}}=\text{O}$ <p>propanal propanoic acid</p> <p>F</p> $\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2\text{Cl}$	<p><i>accept NaOH(alc) if D = acid chloride, Na₂CO₃ (aq).</i></p> <p>Reagent 3 = PCl₅ / SOCl₂ / PCl₃.</p> <p>Reagent 4 = Cr₂O₇²⁻ / H⁺ or MnO₄⁻ / (H⁺) / Fehling / Benedicts/ Tollens</p> <p><i>or if D is given as acid chloride, accept PCl₅ / SOCl₂ / PCl₃ / methanol or other alcohol + acid to give ester in D.</i></p>
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8) i)

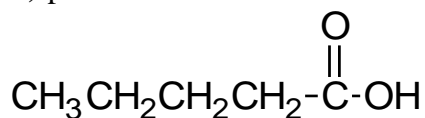


ii) Substitution, the alcohol group is removed and substituted with the chlorine side chain.

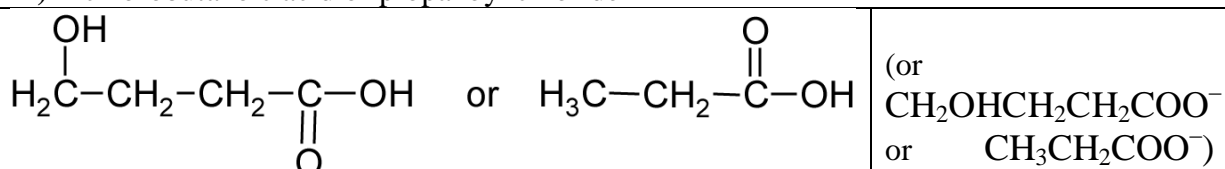
9) i) 4-chlorobutanoic acid



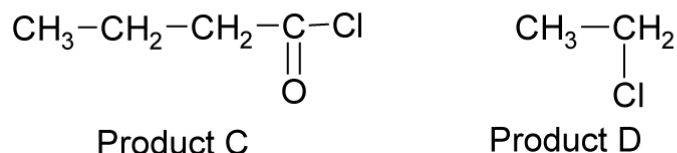
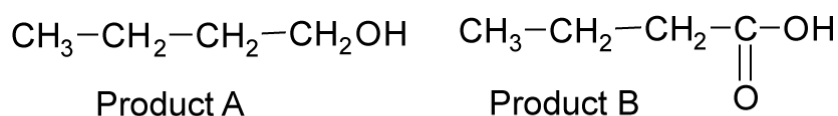
ii) pentanal



iii) 4-chlorobutanoic acid or propanoyl chloride

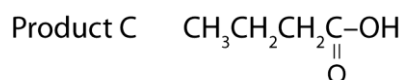
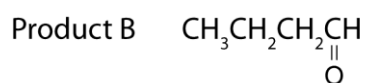


10) Reagent 1 $\text{H}^+ / \text{Cr}_2\text{O}_7^{2-}$ OR $\text{MnO}_4^- / \text{H}^+$ OR MnO_4^-
 Reagent 2 $\text{PCl}_3 / \text{PCl}_5 / \text{SOCl}_2$ OR HBr OR SOBr_2
 Reagent 3 $\text{PCl}_3 / \text{PCl}_5 / \text{SOCl}_2 / \text{conc HCl with ZnCl}_2$ (not just conc HCl)
 Reagent 4 NH_3 (alcohol not required)



Alternative answer:

Reagent 1 (as above) and Reagent 2 = Reagent 1 OR Tollens / Benedicts / Fehlings



11) Aldehyde (propanal) is obtained by heating a mixture of propan-1-ol with acidified (potassium dichromate) solution or (acidified) permanganate solution. Propanal can be removed from the solution as it forms, using distillation, as the aldehyde has a lower boiling point than propan-1-ol and the carboxylic acid. Carboxylic acid (propanoic acid) is obtained by reacting a mixture of propan-1-ol with acidified potassium dichromate solution (under reflux conditions) until all of the reactant has been converted to propanoic acid.

12)

Reagent	Formula
1	PCl_3 , or PCl_5 , or SOCl_2 , or HCl
2	NH_3
3	$\text{Cr}_2\text{O}_7^{2-} / \text{H}^+$ or $\text{MnO}_4^- / \text{H}^+$
4	PCl_3 , or PCl_5 , or SOCl_2
5	CH_3NH_2

Product	Name or formula
1	$\text{H}_3\text{C--CH}_2\text{--CH}_2\text{--CH}_2\text{--Cl}$
2	$\text{H}_3\text{C--CH}_2\text{--CH}_2\text{--}\overset{\text{O}}{\underset{\text{OH}}{\text{C}}}$
3	$\text{H}_3\text{C--CH}_2\text{--CH}_2\text{--}\overset{\text{O}}{\underset{\text{Cl}}{\text{C}}}$

OR

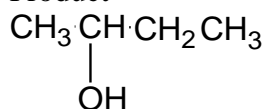
Reagent	Formula
1	PCl ₃ , or PCl ₅ , or SOCl ₂ , or conc HCl
2	NH ₃
3	Cr ₂ O ₇ ²⁻ /H ⁺ or MnO ₄ ⁻ /H ⁺
4	Cr ₂ O ₇ ²⁻ / H ⁺ or MnO ₄ ⁻ /H ⁺
5	CH ₃ NH ₂

Product	Name or formula
1	H ₃ C-CH ₂ -CH ₂ -CH ₂ -Cl
2	H ₃ C-CH ₂ -CH ₂ -C(=O)OH
3	H ₃ C-CH ₂ -CH ₂ -C(=O)H

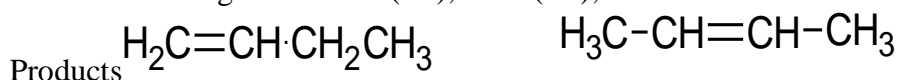
13) Substitution

Reagent NaOH (aq)/ NaOH/ OH⁻ / KOH

Product



Elimination Reagent NaOH (alc), KOH(alc), Ethanolic KOH



OR

cis-but-2-ene and *trans*-but-2-ene

14) i) SOCl₂ / PCl₃ / PCl₅ NOT HCl

ii) CH₃CH₂CH(NH₂)CH₃

Accept recognition that substitution will not occur under these conditions alone.

iii) Reagent 1 Cr₂O₇²⁻ / H⁺ or MnO₄⁻ / H⁺

Product CH₃COOH

Reagent 2 NaOH, Na₂CO₃, NaHCO₃

iv) Reagent 1 conc H₂SO₄

Product CH₃CH=CH₂

Reagent 2 Dilute H₂SO₄ or H⁺ / H₂O

15)

Reaction	Type	Reagent
1	Elimination / Dehydration	conc H ₂ SO ₄
2	Oxidation	Cr ₂ O ₇ ²⁻ / H ⁺ or MnO ₄ ⁻ / H ⁺
3	Substitution	SOCl ₂ , PCl ₃ , PCl ₅ , conc HCl

16) a) i) Reagent 1 – KOH in ethanol/alcohol

Reagent 2 – NaOH(aq) / NaOH/KOH / KOH (aq) / H₂O with OH[–] – *not H₂O*

Reagent 3 – SOCl₂ / PCl₃ / PCl₅ – *not HCl*)

ii) and iii) Compound X (Minor product):

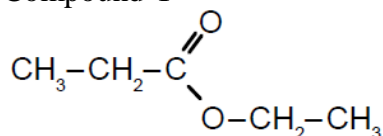
CH₃CH₂CH₂Br or full structure

Name of minor product:

1-bromopropane

CH₃CH₂COCl is propanoyl chloride

Compound Y



OR

CH₃CH₂COOCH₂CH₃ or full structure

Name: ethyl propanoate

b)

(i) Elimination	The molecule HCl / a Cl atom and an H atom removed and a double bond is created.
(ii) Substitution	Br [–] / Br; is removed and replaced / exchanged /swapped with /changed for / substituted with; an OH [–] /OH group.
(iii) Oxidation	Oxygen is added / hydrogen is removed / electrons are lost / the number of bonds to oxygen is increased / the oxidation number of carbon increases / Cr ₂ O ₇ ^{2–} is an oxidising agent / Cr ₂ O ₇ ^{2–} is reduced to Cr ³⁺ so the alcohol is oxidised.

c) If the major product (2-bromopropane) remains in the flask when reagent 2 (NaOH(aq)) is added, a substitution reaction would cause the formation of the 2° alcohol propan-2-ol (CH₃CH(OH)CH₃) as well as propan-1-ol) This would in turn be oxidised by the dichromate to the ketone/ propanone/ (CH₃COCH₃). No further reaction with reagent 3 or ethanol will occur, so the final mixture would contain a lot of propanone and a smaller amount of the ester.

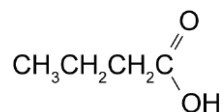
(If all of the alcohol was not completely oxidised to the ketone, an ester with the ester group attached at the 2nd C atom might form with the propanoic acid and 2-chloropropane might result from excess propan-2-ol reacting with reagent 3.)

17)

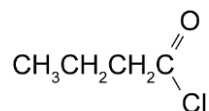
PRODUCTS (letters) REAGENTS (numbers)

1 $\text{Cr}_2\text{O}_7^{2-} / \text{H}^+$ (or $\text{MnO}_4^- / \text{H}^+$)

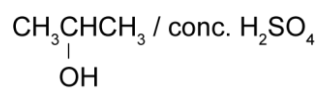
A



B



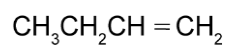
2



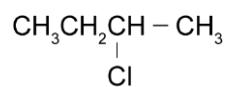
3

conc. H_2SO_4

C



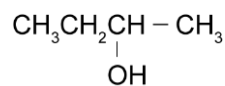
D



4

KOH / NaOH

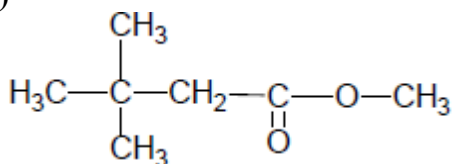
E



5

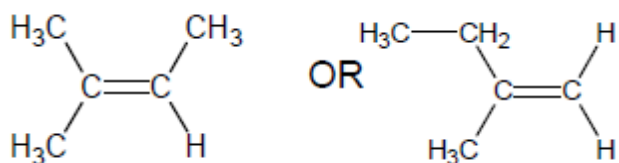
$\text{Cr}_2\text{O}_7^{2-} / \text{H}^+$ (or $\text{MnO}_4^- / \text{H}^+$)

18) i)



condensation /esterification/substitution

ii)



elimination